PERGAMON

Book review

Numerical Simulation of Reactive Flow in Hot Aquifers
Christoph Clauser (Ed.); Springer-Verlag, Berlin, Heidelberg, New York, ISBN 3-540-43868-8, hard back, €169-95, US$179, 332 pages

The conventional approach to geothermal reservoir simulation involves modeling of coupled fluid flow and heat transfer. In recent years there has been increasing interest in considering rock-fluid interaction processes as well. Chemical reactions between minerals and aqueous fluids of different origin and composition can change reservoir porosity and permeability, and may impart a unique chemical signature that can add constraints to reservoir models, increasing their realism and predictive power. The number of fully coupled simulations of thermal–hydrologic–chemical (THC) processes has been limited because software with such capabilities is generally in the research and development stage, and has not been readily available to the practicing reservoir engineer. Enter SHEMAT, a new simulator for non-isothermal flows, with associated solute transport effects and chemical interactions between rocks and fluids. SHEMAT has been developed over a number of years by Christoph Clauser and his associates at the University of Aachen (Germany), and has been applied to a broad array of geothermal reservoir problems.

The handsomely designed book that is the subject of this review is a user's guide to the SHEMAT simulation program. It comes with a CD that includes point-and-click software for installing SHEMAT on PCs. A professional Windows-based user interface for pre- and post-processing with dialog boxes, graphics capabilities, and various utility programs is also included. The book offers a lot more than would be expected from a user's guide for a computer program. It includes much useful information and discussion of current ideas on reactive non-isothermal flows. Especially interesting and valuable, for prospective SHEMAT users as well as for readers with a general interest in chemically reactive flows, is a series of sample problems. A large number of authors have contributed seven different simulation problems that represent their own recent research. These can serve as templates for the development of new SHEMAT applications, as well as illustrating state-of-the-art modeling approaches.

The physical and chemical processes simulated by SHEMAT include single-phase fluid flow, heat transport by conduction and convection, solute diffusion, hydro-dynamic dispersion (approximated as isotropic and Fickian), and chemical reactions between aqueous solutes and mineral phases. The code has options to run only subsets of these processes. Chief application areas include liquid-dominated

geothermal systems, hot dry rock systems, hydrothermal behavior and evolution on a basin scale, and laboratory flow experiments.

SHEMAT uses finite differences for space and time discretization. It is applicable to 2-D and 3-D Cartesian systems, as well as to 2-D cylindrically symmetric grids. In addition to the customary single-point upstream weighting scheme, two alternative higher-order schemes are available for more accurate discretization of the advection term. The algebraic equations resulting from discretization can be solved explicitly, implicitly, or semi-implicitly. The linear equations arising for implicit or semi-implicit time weighting are solved iteratively by the strongly implicit procedure (SIP).

Noteworthy features of SHEMAT include a Pitzer activity model for solutions with high ionic strength, and correlations for permeability change during precipitation and dissolution processes that are based on fractal pore space concepts. Specific calibrations available for major sandstones found in the North German Basin will be useful for analyses in this and similar geologic provinces. SHEMAT can run to high temperatures and pressures. A sample problem investigating magmatic intrusions in the Long Valley Caldera, California, reaches temperatures in excess of 1000 °C. No specific pressure limitation is given, but some of the application examples extend to depths of 20 km and more. Rock thermal conductivity can be specified as a function temperature, as is appropriate for a simulator that can cover such a wide temperature range.

SHEMAT can handle "big" problems. Several of the sample problems have 80,000 nodes or more; the biggest problem presented has 220,000 nodes. A 3-D problem is also included. Users need to be cautioned that running times for some of the problems can be up to several days or weeks on current PCs.

The CD included with the book makes installation of SHEMAT on PCs a very easy and quick process. A detailed tutorial and an array of ready-to-run sample problems are very helpful for getting new users started. The user interface is well designed and powerful. It will take some time for new users to become familiar, which is not surprising given the advanced process modeling capabilities and user features of SHEMAT. The CD also provides a list of SHEMAT users with contact information, inviting and facilitating information exchange.

The publisher maintains a website (http://link.springer.de/software/shemat/ reg_form.htm) where future updates of SHEMAT will be posted. A soon-to-be-released update will allow modeling of freezing and thawing of formation water, which will be useful in the study of permafrost problems.

SHEMAT is not applicable to two-phase liquid-gas systems. However, the code can model dissolved CO_2. As shown in two figures (Figs. 4.1.6, 7), CO_2 solubility has a realistic dependence on temperature and salinity. Neither the text nor the figure captions spell out the pressure conditions for which solubilities are plotted (our tests indicate that total pressure is $P_{tot} = 1$ atm $= 1.013$ bar, so that CO_2 partial pressure is $P_{CO_2} = P_{tot} - P_{sat}$, with P_{sat} the saturated vapor pressure of the brine). Mineral precipitation and dissolution can be modeled by local equilibrium or kinetic rates, but the choice made here applies to all minerals in the simulation. It would be desirable to provide more flexibility by allowing some minerals to be at equilibrium,

such as calcite and anhydrite, while other mineral reactions may proceed very slowly and are kinetically controlled, such as precipitation of quartz or amorphous silica. The SHEMAT database includes the main anions and cations found in hydrothermal systems, but some commonly encountered minerals such as alumosilicates are not available. The subject index is very brief and therefore not very helpful.

In spite of the limitations just mentioned, SHEMAT is a powerful simulation program that is applicable to a broad range of geothermal reservoir problems. The array of test problems provided with the code is very impressive and informative. SHEMAT with its comprehensive user's guide is a very welcome and timely addition to the toolbox of the practicing reservoir engineer.

Karsten Pruess, Tianfu Xu
Lawrence Berkeley National Laboratory,
Berkeley, CA 94720, USA
E-mail address: k_pruess@lbl.gov